Fullerenes with distant pentagons

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Abstract

For each $d > 0$, we find all the smallest fullerenes for which the least distance between two pentagons is d. We also show that for each d there is an h_d such that fullerenes with pentagons at least distance d apart and any number of hexagons greater than or equal to h_d exist.

We also determine the number of fullerenes where the minimum distance between any two pentagons is at least d, for $1 \leq d \leq 5$, up to 400 vertices.

1 Introduction

A *fullerene* [12] is a cubic plane graph where all faces are pentagons or hexagons. Euler's formula implies that a fullerene with n vertices contains exactly 12 pentagons and $n/2-10$ hexagons.

The *dual* of a fullerene is the plane graph obtained by exchanging the roles of vertices and faces: the vertex set of the dual graph is the set of faces of the original graph and two vertices in the dual graph are adjacent if and only if the two faces share an edge in the original graph.

The dual of a fullerene with n vertices is a *triangulation* (i.e. a plane graph where every face is a triangle) which contains 12 vertices with degree 5 and $n/2 - 10$ vertices with degree 6. The *face-distance* between two pentagons is the distance between the corresponding vertices of degree 5 in the dual graph.

The first fullerene molecule (i.e. the C_{60} "buckyball") was discovered in 1985 by Kroto et al. [12]. Among the fullerenes, the *Isolated Pentagon Rule* (IPR) fullerenes are of special interest as they tend to be more stable [1, 16]. IPR fullerenes are fullerenes where no two pentagons share an edge, i.e. they have minimum face-distance at least 2. Raghavachari [13] argued that steric strain will be minimized when the pentagons are distributed as uniformly as possible and therefore proposed the *uniform curvature rule* as an extension of the IPR rule. Also, more recently Rodríguez-Fortea et al. [14] proposed the maximum pentagon separation rule where they argue that the most suitable carbon cages are those with the largest separations among the 12 pentagons. These observations lead us to investigate the maximum separation between pentagons that can be achieved for a given number of atoms, or conversely how many atoms are needed to achieve a given separation. We will refer to the least face-distance between pentagons of a fullerene as the *pentagon separation* of the fullerene.

In the next section we determine the smallest fullerenes with a given pentagon separation. We also show that the minimum fullerenes for each d are unique up to mirror image and that for each d there is an h_d such that fullerenes with pentagon separation at least d and any number of hexagons greater than or equal to h_d exist. The latter was already proven for h_1 (i.e., for all fullerenes) by Grünbaum and Motzkin in [10] and for h_2 (i.e., for IPR fullerenes) by Klein and Liu in [11].

Finally, we also determine the number of fullerenes of pentagon separation d, for $1 \leq d \leq 5$, up to 400 vertices.

2 Fullerenes with a given minimum pentagon separation

In this section we determine the smallest fullerenes with a given pentagon separation.

We remind the reader of the icosahedral fullerenes [5,9]. These fullerenes are uniquely determined by their Coxeter coordinates (p, q) and are obtained by cutting an equilateral Goldberg triangle with coordinates (p, q) from the hexagon lattice and gluing it to the faces of the icosahedron. As a Goldberg triangle with coordinates (p, q) has $p^2 + pq + q^2$ vertices, an icosahedral fullerene with Coxeter coordinates (p, q) has $20(p^2 + pq + q^2)$ vertices. Also note that an icosahedral fullerene with Coxeter coordinates (p, q) has pentagon separation $p + q$.

The smallest fullerene for $d = 1$ is of course unique: the icosahedron C_{20}. For larger d, the minimal fullerenes are given in the next theorem.

Theorem 2.1. *For odd $d \geq 3$, the smallest fullerenes with pentagon separation at least d are the icosahedral fullerenes with Coxeter coordinates $(\lceil d/2 \rceil, \lfloor d/2 \rfloor)$ and $(\lfloor d/2 \rfloor, \lceil d/2 \rceil)$. These are mirror images and have $15d^2 + 5$ vertices. For even d, the unique smallest fullerene with pentagon separation at least d is the the icosahedral fullerene with Coxeter coordinates $(d/2, d/2)$, which has $15d^2$ vertices.*

Proof.

Proof in the case that $d \geq 3$ is odd:

The *penta-hexagonal net* is the regular tiling of the plane where a central pentagon is surrounded by an infinite number of hexagons. The number of faces at face-distance k from the pentagon in the penta-hexagonal net is $5k$. So the number of faces at face-distance at most k from the pentagon in the penta-hexagonal net is $\sum_{i=1}^{k} 5i + 1 = 5k(k+1)/2 + 1$. Figure 1 shows this situation for $k = 3$.

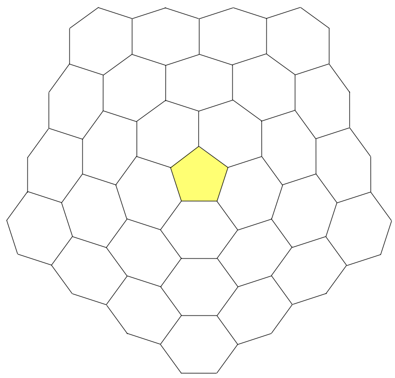

Figure 1: Patch for $d = 7$ in the proof of Theorem 2.1

In a fullerene with pentagon separation at least d, for odd d, the sets of faces at face-distance at most $\lfloor d/2 \rfloor$ from each pentagon are pairwise disjoint. Consequently the smallest such fullerenes we can hope to find consist of 12 copies of the above patch for $k = \lfloor d/2 \rfloor$, which comes to $15d^2 + 5$ vertices.

Since the patch boundary has no more than two consecutive vertices of degree 2, it is impossible to join any number of them into a larger patch with a boundary having more than two consecutive vertices of degree 2. Therefore, considering the complement, no union of these patches which is completable to a fullerene has more than two consecutive vertices of degree 3. Now, every way to overlap the boundaries of two patches produces

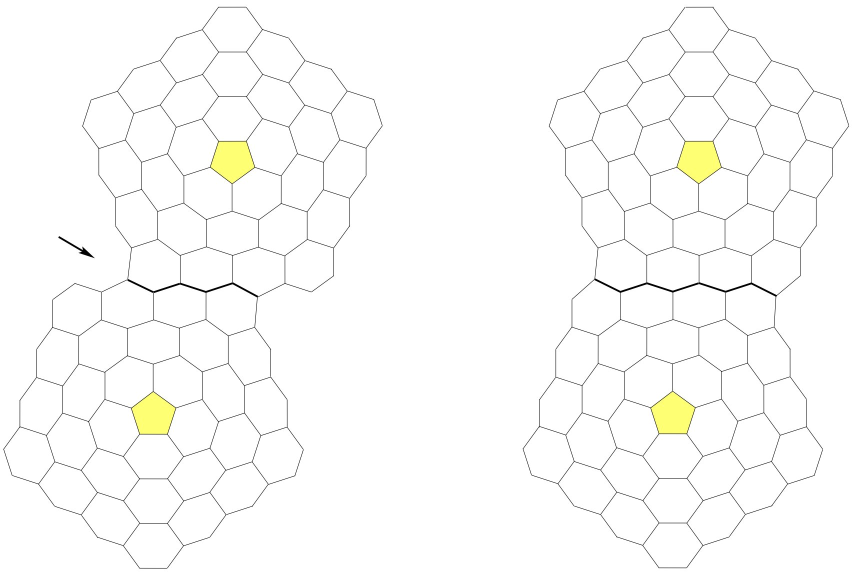

Figure 2: Bad and good ways to join two patches for $d = 7$

three consecutive vertices of degree 3, such as indicated in the left side of Figure 2, except for the way shown in the right side of Figure 2 or its mirror image. For each of these two starting points, there is only one way to attach a third patch to those two patches, and so on, leading to a unique completion in each case. It is easy to see that these two fullerenes are the icosahedral fullerenes mentioned in the theorem.

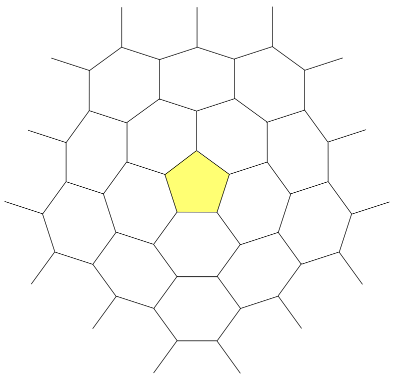

Figure 3: Patch with dangling edges for $d = 6$ in the proof of Theorem 2.1

Proof in the case that d is even:

The proof in this case is similar except that we use a different type of patch. In [6] it was proven that the number of vertices at distance k from the pentagon in the penta-hexagonal net is $5\lfloor k/2 \rfloor + 5$. So the total number of vertices at distance at most k from the pentagon in the penta-hexagonal net is $\sum_{i=0}^{k}(5\lfloor i/2 \rfloor + 5) = 5(\sum_{i=0}^{k}\lfloor i/2 \rfloor + k + 1)$. If k is even, $\sum_{i=0}^{k}\lfloor i/2 \rfloor$ is equal to $k^2/4$. So the total number of vertices at distance at most k from the pentagon in the penta-hexagonal net for even k is $5(k^2/4 + k + 1)$.

In a fullerene with pentagon separation at least d, for even d, the sets of vertices at distance at most $d-2$ from every pentagon are pairwise disjoint. The case of $d=6$ is shown in Figure 3, excluding the ends of the dangling edges. Therefore, the smallest such fullerene of pentagon separation d we can hope to construct consists of 12 of these patches for $k=d-2$, joined together by identifying dangling edges. This would give us $15d^2$ vertices altogether.

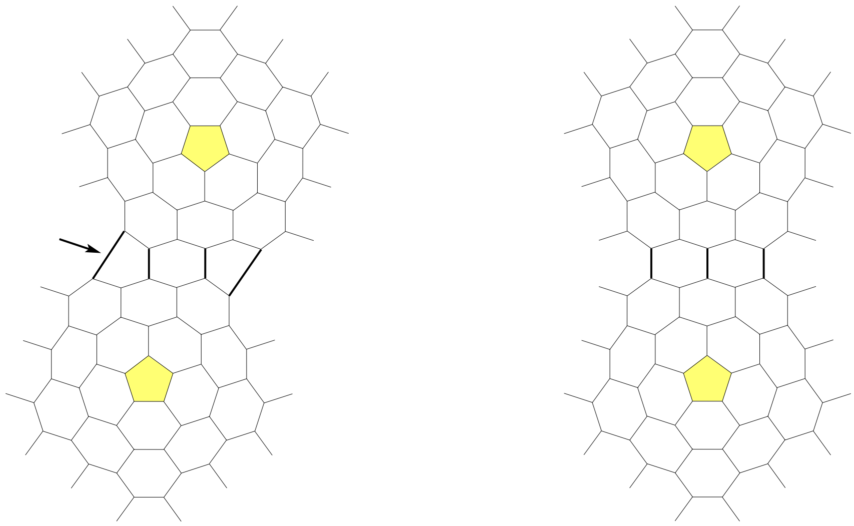

Figure 4: Bad and good ways to identify dangling edges for $d=6$

Since we are only permitted to create hexagons incident with the dangling edges, dangling edges distance two apart in one patch can only be identified with dangling edges distance two apart in another patch. Otherwise, a face of the wrong size is created, such as the pentagon indicated in the left side of Figure 4. This allows us to join two adjacent patches in only one way, as shown by the right side of Figure 4. Extra patches can then be attached in unique fashion, leading to a single fullerene that is easily seen to be the icosahedral fullerene with Coxeter coordinates $(d/2, d/2)$. □

Next we will prove that for each d there is an h_d such that fullerenes with pentagon separation at least d and any number of hexagons greater than or equal to h_d exist. To prove this, we need Lemmas 2.2 and 2.3.

A *fullerene patch* is a connected subgraph of a fullerene where all faces except one exterior face are also faces in the fullerene and all boundary vertices have degree 2 or 3 and all non-boundary vertices have degree 3. The *boundary sequence* of a patch is the cyclic sequence of the degrees of the vertices in the boundary of a patch in clockwise or counterclockwise order.

A *cap* is a fullerene patch which contains 6 pentagons and has a boundary sequence of the form $(23)^l(32)^m$. Such a boundary is represented by the parameters (l,m). In the literature, the vector (l,m) is also called the *chiral vector* (see [15]).

Lemma 2.2. *Any cap with parameters* $(l,0)$ *can be transformed into a cap with parameters* $(l,1)$ *without decreasing the minimum face-distance between the pentagons of the cap.*

Proof. Given a cap with parameters $(l,0)$. If the cap does not contain a pentagon in its boundary, we remove $(l,0)$ rings of hexagons until there is a pentagon in the boundary of the cap.

In Figure 5 we show how the $(l,0)$ cap which contains a boundary pentagon (see Figure 5a) can be transformed into a cap with parameters $(l,1)$ without decreasing the minimum face-distance between the pentagons. This is done by changing the boundary pentagon into a hexagon h, adding a ring of hexagons (see Figure 5b) and changing a hexagon in the boundary which is adjacent to h into a pentagon (see Figure 5c). □

Lemma 2.3. *Given a cap* C *with parameters* (l,m) *with* $l \neq 0$ *and* $m \neq 0$ *and which consists of* f *faces. A cap* C' *with the same parameters* (l,m) *which contains* C *as a subgraph and has* $f+l$*, respectively* $f+m$ *faces can be constructed from* C *by adding* l *or* m *hexagons to* C*, respectively.*

Proof. Given a cap C with parameters (l,m) with $l \neq 0$ and $m \neq 0$. In Figure 6 we show how a cap C' with the same parameters (l,m) which contains C as a subgraph and has $f+l$ faces can be constructed from C by adding l hexagons to C.

A cap C'' with $f+m$ faces can be obtained in a completely analogous way by adding m hexagons to C. □

Theorem 2.4. *For each* d *there is an* h_d *such that fullerenes with pentagon separation at least* d *and any number of hexagons greater than or equal to* h_d *exist.*

Proof. Given an icosahedral fullerene F with Coxeter coordinates $(\lceil d/2 \rceil, \lceil d/2 \rceil)$. In this fullerene the minimum face-distance between the pentagons is $2\lceil d/2 \rceil$.

Brinkmann and Schein [4] have proven that every icosahedral fullerene with Coxeter coordinates (p,q) contains a fullerene patch with 6 pentagons which is a subgraph of a cap with parameters $(3(p+2q), 3(p-q))$. So F contains a fullerene patch with 6 pentagons which is a subgraph of a cap with parameters $(9\lceil d/2 \rceil, 0)$.

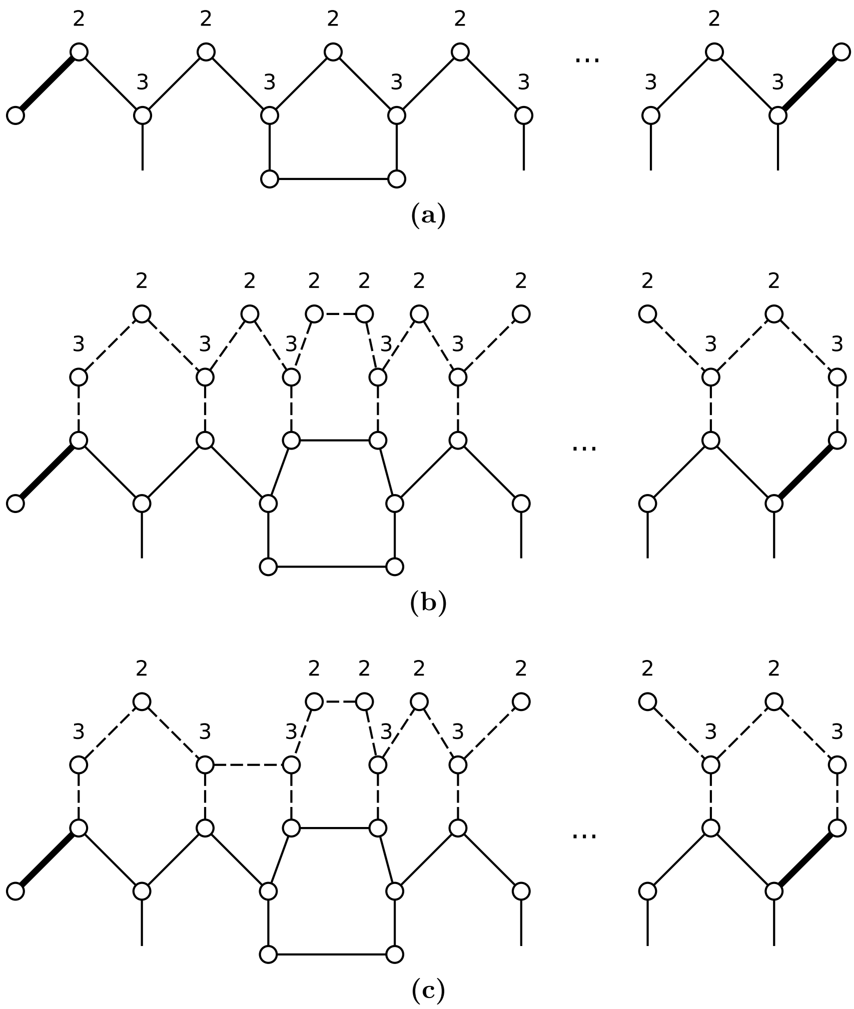

Figure 5: Procedure to change a cap with parameters $(l, 0)$ to a cap with parameters $(l, 1)$. The bold edges in the figure have to be identified with each other.

It follows from [7, 15] that such a fullerene patch can be completed to a cap with parameters $(9\lceil d/2\rceil, 0)$ by adding hexagons. It follows from Lemma 2.2 that this cap can then be transformed to a cap with parameters $(9\lceil d/2\rceil, 1)$ without decreasing the minimum face-distance between the pentagons of the cap.

We form a fullerene F' with pentagon separation at least d by gluing together two copies of the $(9\lceil d/2\rceil, 1)$ cap and adding $(9\lceil d/2\rceil, 1)$ rings of hexagons if necessary. Let $h_{F'}$ denote the number of hexagons of F'. Now a fullerene with pentagon separation at least d and any number of hexagons greater than $h_{F'}$ can be obtained by recursively applying Lemma 2.3 to F'. $\square$

The counts of the number of fullerenes up to 400 vertices with pentagon separation at least d, for $1 \leq d \leq 5$, can be found in Tables 1-4. (Note that $d = 1$ gives the set of all fullerenes and $d = 2$ gives the set of all IPR fullerenes). These counts were

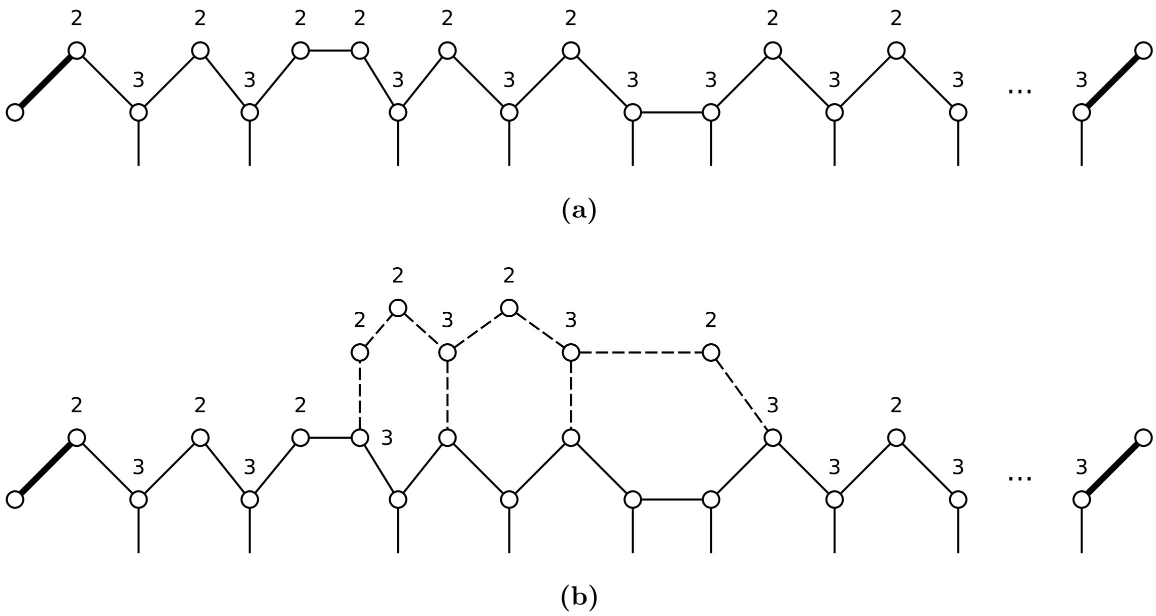

Figure 6: Procedure which adds l hexagons to an (l, m) cap without changing the boundary parameters. The bold edges in the figure have to be identified with each other.

obtained by using the program *buckygen* [3, 8] (which can be downloaded from `http://caagt.ugent.be/buckygen/`) to generate all non-isomorphic IPR fullerenes and then applying a separate program to compute their pentagon separation. Note that fullerenes which are mirror images of each other are considered to be in the same isomorphism class and are thus only counted once.

Some of the fullerenes from Tables 1-4 can also be downloaded from the *House of Graphs* [2] at `http://hog.grinvin.org/Fullerenes` . Figures 7-9 show the smallest fullerenes with pentagon separation d, for $3 \leq d \leq 5$.

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References

[1] E. Albertazzi, C. Domene, P.W. Fowler, T. Heine, G. Seifert, C. Van Alsenoy, and F. Zerbetto. Pentagon adjacency as a determinant of fullerene stability. *Physical Chemistry Chemical Physics*, 1(12):2913–2918, 1999.

nv	nf	fullerenes	IPR fullerenes	pent. sep. ≥ 3	pent. sep. ≥ 4	pent. sep. ≥ 5
20	12	1	0	0	0	0
22	13	0	0	0	0	0
24	14	1	0	0	0	0
26	15	1	0	0	0	0
28	16	2	0	0	0	0
30	17	3	0	0	0	0
32	18	6	0	0	0	0
34	19	6	0	0	0	0
36	20	15	0	0	0	0
38	21	17	0	0	0	0
40	22	40	0	0	0	0
42	23	45	0	0	0	0
44	24	89	0	0	0	0
46	25	116	0	0	0	0
48	26	199	0	0	0	0
50	27	271	0	0	0	0
52	28	437	0	0	0	0
54	29	580	0	0	0	0
56	30	924	0	0	0	0
58	31	1 205	0	0	0	0
60	32	1 812	1	0	0	0
62	33	2 385	0	0	0	0
64	34	3 465	0	0	0	0
66	35	4 478	0	0	0	0
68	36	6 332	0	0	0	0
70	37	8 149	1	0	0	0
72	38	11 190	1	0	0	0
74	39	14 246	1	0	0	0
76	40	19 151	2	0	0	0
78	41	24 109	5	0	0	0
80	42	31 924	7	0	0	0
82	43	39 718	9	0	0	0
84	44	51 592	24	0	0	0
86	45	63 761	19	0	0	0
88	46	81 738	35	0	0	0
90	47	99 918	46	0	0	0
92	48	126 409	86	0	0	0
94	49	153 493	134	0	0	0
96	50	191 839	187	0	0	0
98	51	231 017	259	0	0	0
100	52	285 914	450	0	0	0
102	53	341 658	616	0	0	0
104	54	419 013	823	0	0	0
106	55	497 529	1 233	0	0	0
108	56	604 217	1 799	0	0	0
110	57	713 319	2 355	0	0	0
112	58	860 161	3 342	0	0	0
114	59	1 008 444	4 468	0	0	0

Table 1: Number of fullerenes for a given lower bound on the pentagon separation. nv is the number of vertices and nf is the number of faces.

nv	nf	fullerenes	IPR fullerenes	pent. sep. ≥ 3	pent. sep. ≥ 4	pent. sep. ≥ 5
116	60	1 207 119	6 063	0	0	0
118	61	1 408 553	8 148	0	0	0
120	62	1 674 171	10 774	0	0	0
122	63	1 942 929	13 977	0	0	0
124	64	2 295 721	18 769	0	0	0
126	65	2 650 866	23 589	0	0	0
128	66	3 114 236	30 683	0	0	0
130	67	3 580 637	39 393	0	0	0
132	68	4 182 071	49 878	0	0	0
134	69	4 787 715	62 372	0	0	0
136	70	5 566 949	79 362	0	0	0
138	71	6 344 698	98 541	0	0	0
140	72	7 341 204	121 354	1	0	0
142	73	8 339 033	151 201	0	0	0
144	74	9 604 411	186 611	0	0	0
146	75	10 867 631	225 245	0	0	0
148	76	12 469 092	277 930	0	0	0
150	77	14 059 174	335 569	1	0	0
152	78	16 066 025	404 667	2	0	0
154	79	18 060 979	489 646	0	0	0
156	80	20 558 767	586 264	0	0	0
158	81	23 037 594	697 720	0	0	0
160	82	26 142 839	836 497	2	0	0
162	83	29 202 543	989 495	1	0	0
164	84	33 022 573	1 170 157	2	0	0
166	85	36 798 433	1 382 953	1	0	0
168	86	41 478 344	1 628 029	13	0	0
170	87	46 088 157	1 902 265	4	0	0
172	88	51 809 031	2 234 133	12	0	0
174	89	57 417 264	2 601 868	10	0	0
176	90	64 353 269	3 024 383	28	0	0
178	91	71 163 452	3 516 365	23	0	0
180	92	79 538 751	4 071 832	58	0	0
182	93	87 738 311	4 690 880	54	0	0
184	94	97 841 183	5 424 777	142	0	0
186	95	107 679 717	6 229 550	129	0	0
188	96	119 761 075	7 144 091	291	0	0
190	97	131 561 744	8 187 581	257	0	0
192	98	145 976 674	9 364 975	548	0	0
194	99	159 999 462	10 659 863	566	0	0
196	100	177 175 687	12 163 298	1 126	0	0
198	101	193 814 658	13 809 901	1 072	0	0
200	102	214 127 742	15 655 672	1 943	0	0
202	103	233 846 463	17 749 388	2 080	0	0
204	104	257 815 889	20 070 486	3 682	0	0
206	105	281 006 325	22 606 939	3 992	0	0
208	106	309 273 526	25 536 557	6 340	0	0
210	107	336 500 830	28 700 677	6 737	0	0

Table 2: Number of fullerenes for a given lower bound on the pentagon separation (continued). nv is the number of vertices and nf is the number of faces.

nv	nf	fullerenes	IPR fullerenes	pent. sep. ≥ 3	pent. sep. ≥ 4	pent. sep. ≥ 5
212	108	369 580 714	32 230 861	10 513	0	0
214	109	401 535 955	36 173 081	12 000	0	0
216	110	440 216 206	40 536 922	18 169	0	0
218	111	477 420 176	45 278 722	20 019	0	0
220	112	522 599 564	50 651 799	28 528	0	0
222	113	565 900 181	56 463 948	32 276	0	0
224	114	618 309 598	62 887 775	46 534	0	0
226	115	668 662 698	69 995 887	52 177	0	0
228	116	729 414 880	77 831 323	71 303	0	0
230	117	787 556 069	86 238 206	79 915	0	0
232	118	857 934 016	95 758 929	109 848	0	0
234	119	925 042 498	105 965 373	124 153	0	0
236	120	1 006 016 526	117 166 528	164 700	0	0
238	121	1 083 451 816	129 476 607	184 404	0	0
240	122	1 176 632 247	142 960 479	242 507	1	0
242	123	1 265 323 971	157 402 781	273 885	0	0
244	124	1 372 440 782	173 577 766	353 997	0	0
246	125	1 474 111 053	190 809 628	397 673	0	0
248	126	1 596 482 232	209 715 141	507 913	0	0
250	127	1 712 934 069	230 272 559	570 053	0	0
252	128	1 852 762 875	252 745 513	717 983	0	0
254	129	1 985 250 572	276 599 787	805 374	0	0
256	130	2 144 943 655	303 235 792	1 007 680	0	0
258	131	2 295 793 276	331 516 984	1 127 989	0	0
260	132	2 477 017 558	362 302 637	1 392 996	2	0
262	133	2 648 697 036	395 600 325	1 550 580	0	0
264	134	2 854 536 850	431 894 257	1 905 849	0	0
266	135	3 048 609 900	470 256 444	2 124 873	1	0
268	136	3 282 202 941	512 858 451	2 592 104	1	0
270	137	3 501 931 260	557 745 670	2 868 467	2	0
272	138	3 765 465 341	606 668 511	3 461 487	1	0
274	139	4 014 007 928	659 140 287	3 847 594	0	0
276	140	4 311 652 376	716 217 922	4 621 524	1	0
278	141	4 591 045 471	776 165 188	5 112 067	2	0
280	142	4 926 987 377	842 498 881	6 079 570	4	0
282	143	5 241 548 270	912 274 540	6 726 996	1	0
284	144	5 618 445 787	987 874 095	7 971 111	10	0
286	145	5 972 426 835	1 068 507 788	8 784 514	3	0
288	146	6 395 981 131	1 156 161 307	10 352 546	7	0
290	147	6 791 769 082	1 247 686 189	11 385 724	9	0
292	148	7 267 283 603	1 348 832 364	13 357 318	5	0
294	149	7 710 782 991	1 454 359 806	14 652 198	6	0
296	150	8 241 719 706	1 568 768 524	17 102 231	24	0
298	151	8 738 236 515	1 690 214 836	18 756 139	16	0
300	152	9 332 065 811	1 821 766 896	21 766 152	32	0
302	153	9 884 604 767	1 958 581 588	23 815 310	36	0
304	154	10 548 218 751	2 109 271 290	27 529 516	46	0
306	155	11 164 542 762	2 266 138 871	30 090 574	54	0

Table 3: Number of fullerenes for a given lower bound on the pentagon separation (continued). nv is the number of vertices and nf is the number of faces.

nv	nf	fullerenes	IPR fullerenes	pent. sep. ≥ 3	pent. sep. ≥ 4	pent. sep. ≥ 5
308	156	11 902 015 724	2 435 848 971	34 629 672	99	0
310	157	12 588 998 862	2 614 544 391	37 770 691	93	0
312	158	13 410 330 482	2 808 510 141	43 312 313	135	0
314	159	14 171 344 797	3 009 120 113	47 153 778	187	0
316	160	15 085 164 571	3 229 731 630	53 899 686	211	0
318	161	15 930 619 304	3 458 148 016	58 585 441	308	0
320	162	16 942 010 457	3 704 939 275	66 712 070	443	0
322	163	17 880 232 383	3 964 153 268	72 395 888	535	0
324	164	19 002 055 537	4 244 706 701	82 171 212	698	0
326	165	20 037 346 408	4 533 465 777	89 063 353	1 026	0
328	166	21 280 571 390	4 850 870 260	100 785 130	1 216	0
330	167	22 426 253 115	5 178 120 469	109 068 073	1 623	0
332	168	23 796 620 378	5 531 727 283	122 992 213	2 489	0
334	169	25 063 227 406	5 900 369 830	132 950 223	2 788	0
336	170	26 577 912 084	6 299 880 577	149 523 121	3 612	0
338	171	27 970 034 826	6 709 574 675	161 430 830	4 744	0
340	172	29 642 262 229	7 158 963 073	181 076 418	5 845	0
342	173	31 177 474 996	7 620 446 934	195 124 334	7 457	0
344	174	33 014 225 318	8 118 481 242	218 323 289	10 591	0
346	175	34 705 254 287	8 636 262 789	235 050 400	12 307	0
348	176	36 728 266 430	9 196 920 285	262 381 050	15 312	0
350	177	38 580 626 759	9 768 511 147	282 042 413	19 574	0
352	178	40 806 395 661	10 396 040 696	314 052 518	23 755	0
354	179	42 842 199 753	11 037 658 075	337 229 970	29 793	0
356	180	45 278 616 586	11 730 538 496	374 666 300	38 688	0
358	181	47 513 679 057	12 446 446 419	401 932 458	45 946	0
360	182	50 189 039 868	13 221 751 502	445 482 235	55 742	0
362	183	52 628 839 448	14 010 515 381	477 264 068	69 970	0
364	184	55 562 506 886	14 874 753 568	528 016 753	83 616	0
366	185	58 236 270 451	15 754 940 959	565 045 586	100 644	0
368	186	61 437 700 788	16 705 334 454	623 895 236	126 048	0
370	187	64 363 670 678	17 683 643 273	666 935 811	149 044	0
372	188	67 868 149 215	18 744 292 915	734 907 336	179 013	0
374	189	71 052 718 441	19 816 289 281	784 797 263	217 673	0
376	190	74 884 539 987	20 992 425 825	863 237 405	257 673	0
378	191	78 364 039 771	22 186 413 139	920 935 351	302 553	0
380	192	82 532 990 559	23 475 079 272	1 011 152 383	367 547	1
382	193	86 329 680 991	24 795 898 388	1 077 679 749	434 339	0
384	194	90 881 152 117	26 227 197 453	1 181 149 036	507 481	0
386	195	95 001 297 565	27 670 862 550	1 257 630 423	611 532	0
388	196	99 963 147 805	29 254 036 711	1 376 400 812	707 184	0
390	197	104 453 597 992	30 852 950 986	1 463 926 563	820 525	0
392	198	109 837 310 021	32 581 366 295	1 599 524 989	982 532	0
394	199	114 722 988 623	34 345 173 894	1 699 970 613	1 133 377	0
396	200	120 585 261 143	36 259 212 641	1 854 374 011	1 323 509	0
398	201	125 873 325 588	38 179 777 473	1 969 147 856	1 546 304	0
400	202	132 247 999 328	40 286 153 024	2 144 985 583	1 784 313	1

Table 4: Number of fullerenes for a given lower bound on the pentagon separation (continued). nv is the number of vertices and nf is the number of faces.

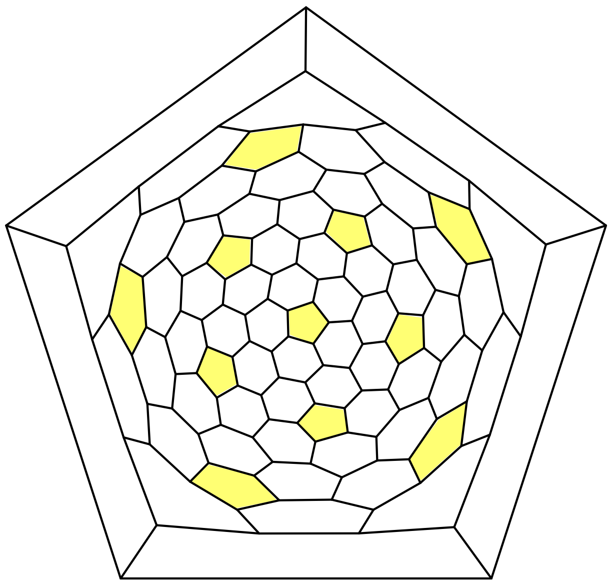

Figure 7: The icosahedral fullerene with Coxeter coordinates $(2, 1)$. This fullerene and its mirror image are the smallest fullerenes with pentagon separation 3. They have 140 vertices.

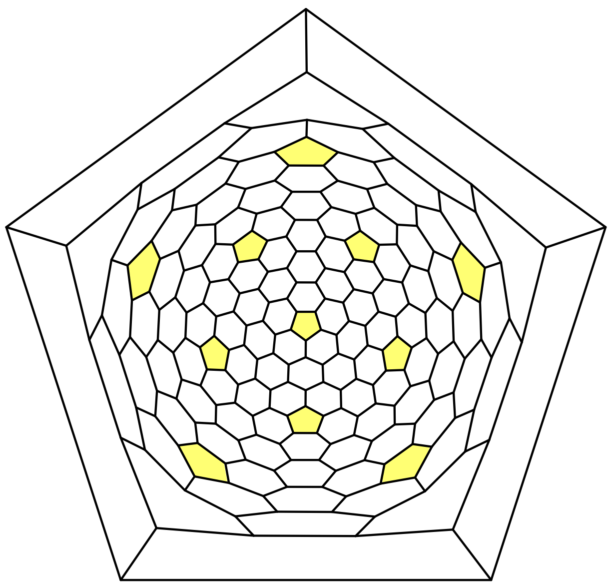

Figure 8: The icosahedral fullerene with Coxeter coordinates $(2, 2)$. This is the smallest fullerene with pentagon separation 4 and has 240 vertices.

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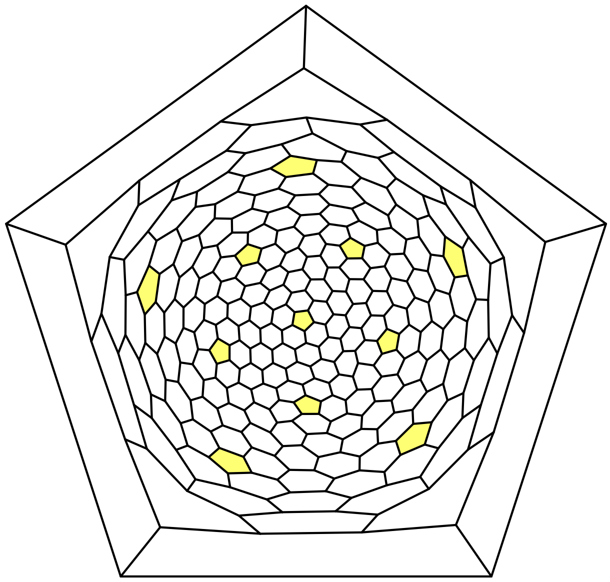

Figure 9: The icosahedral fullerene with Coxeter coordinates $(3, 2)$. This fullerene and its mirror image are the smallest fullerenes with pentagon separation 5. They have 380 vertices.

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